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Frequential and temporal analysis of two-dimensional photonic crystals for absorption enhancement in organic solar cells

L. Peres, V. Vigneras, S. Fasquel *,[1]

University of Bordeaux, IMS, UMR 5218, F-33400 Talence, France

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ABSTRACT

We propose a theoretical study of the role of a two-dimensional photonic crystal in an organic solar cell. In particular, we use some specific resonant modes of the photonic crystal, that are not guided modes, to favor light trapping in the absorbing medium. The increase of optical path in the active layer causes an increase of absorption at some particular frequencies. A frequential-temporal analysis has been made to highlight the correspondence between absorption enhancement and photonic crystal resonant modes, in a thin absorbing slab. In addition we present possible designs that would broaden the absorption spectrum of the bulk material. Finally, we study a complete organic bulk heterojunction solar cell made of a 50 nm-thick active layer, and a patterned ITO electrode. In such device, the well known trade-off between carrier extraction and light absorption can appear as a constraint. Our challenge is to obtain a high absorption in an ultra thin active layer solar cell, by using a light trapping effect.

1. Introduction

Over the last few years a new generation of ultra-thin film solar cells have been studied. Their performances do not only rely on the intrinsic properties of the absorbing materials but also on the way electromagnetic radiation interacts with the whole cell architecture [1]. In this context, recent theoretical and experimental studies have been made on finding ways to enhance the optical absorption in both inorganic and organic solar cells. This can be done with diffraction gratings, to increase the optical path in the absorbing medium [2,3]. Other methods use the plasmonic resonance of noble metal nanoparticles in order to confine the electromagnetic field near the active layer [4–8]. Finally another approach uses the Photonic Crystal (PC) properties of periodically patterned dielectric materials to trap photons and increase their interaction time with the active layer [9–15]. All those different physical mechanisms, employed to enhance absorption in a solar cell, are based on the optical response of nano inclusions or patterns that are present in one or several layers of the solar cell [13,15]. The size and nature of the nano-objects as well as the choice of the patterned layer(s) represent additional degrees of freedom that can be used to find an optimized absorption (under the constraint of technological possibilities), compared to an unpatterned structure.

In this article a photonic crystal approach is used to control the optical behavior of different architectures, and an improvement of the performances of organic bulk heterojunction solar cells [16,17] is proposed. 1D and 2D periodic structures have been studied in different nanopatterned (organic or inorganic) solar cells. Indeed, we can find solar cells with nanopattern in the active layer [11], in the metallic electrode [5], ITO electrode [18], or in both electrode and active layer [15,19]. For both organic and inorganic nanopatterned solar cells, there is a common challenge that is to broaden the absorption spectrum [9,18] in order to increase the solar cell efficiency. To a given layered structure (index of refraction, thicknesses) would correspond an optimized photonic crystal (spacing and diameters of holes) to maximize absorption enhancement at a given wavelength, or, in average, on the whole spectrum.

Due to the differences between organic and inorganic materials, physical mechanism, such as optical absorption and charges transport, are different. This is a reason why photonic crystal challenges are not exactly the same in organic and organic solar cells. In particular in our typical organic bulk heterojunction solar cells, there is a well known trade-off between light absorption and charge transport that appear as a constraint: the higher the thickness the higher the absorption but the higher is the charges recombination in the active layer. So a specific challenge of our works is to use a PC trapping effect leading to high absorption level in a very thin active layer solar cell.

Complete organic solar cells with PC can be quite complex, as they contain several layers of dielectric, structured dielectric, and metal. Thus to point out clearly the essential phenomena, we shall first analyze the role of PC using the simplest possible system: an

* Corresponding author. Tel.:+33 5 40 00 66 30.
E-mail address: sophie.fasquel@ims-bordeaux.fr (S. Fasquel).
[1] Postal address: ENSCBP 16 avenue de Pey-Berland 33 607 Pessac Cedex.

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absorbing slab, structured as a PC (see Fig. 2a), before to study a complete solar cell (see Fig. 6a).

In the first section, we describe the electromagnetic interaction between sunlight and a multilayer solar cell, as well as the associated numerical tools to model it. In the second section, the simulations results will be presented. The section has been split up in two parts: subsection 3.1 describes the photonic crystal (PC) resonance found in a single absorbing slab. An absorption enhancement due to the presence of the PC is pointed out. To explain the physics of the trapping effect and link it to PC resonances, a parametric study is carried out. Then a frequential and temporal analysis is made, so as to link the PC resonant mode and the absorption enhancement.

In subsection 3.2 we use the PC properties of Section 3.1 in a more realistic multilayer solar cell structure. We show that patterning the electrode with a bidimensional PC can increase absorption in the active layer. In this case, the absorbing layer is unpatterned.

2. Numerical methods

We model the electromagnetic interaction between the sun light and a solar cell, made of several layers. Among them there is an active layer – in which excitons are first created then dissociated – and electrodes that harvest the charges. Optically, this multilayered device acts as an interferential system. Thus all the layers parameters have to be taken into account to compute the global optical response and the quantum efficiency.

More precisely, as we want to model the absorption improvements induced by a photonic crystal in a solar cell, we shall include a two-dimensional (2D) array of air holes in our three-dimensionnal (3D) multilayer system. The whole patterned architecture can be modeled by using two different numerical methods that give complementary information: Finite Elements Method (FEM) and Finite Difference Time Domain (FDTD).

To model the coupling between the injected wave and the whole multilayer cell we use 3D methods such as FEM [20] and FDTD [21]. Those two methods solve the exact Maxwell equations, and give as a result the 6 components of the electromagnetic fields (E, H), on a three dimensional grid.

The FEM calculates the spatial field profiles as the response of the system to a particular frequency and boundary condition. With this method, we take into account the dispersion of all materials easily. In this work, all the absorption spectra have been calculated with FEM.

The FDTD method permits to compute the spatio-temporal evolution of a plane wave which is incident on a metallo-dielectric system. In particular we use FDTD in Section 3.1.1 to compute the transient evolution of a field, when light is trapped in a photonic crystal slab.

For both FDTD and FEM, the structures have been designed in 3D space and are excited by a Transverse Electro-Magnetic (TEM) plane wave at normal incidence. The symmetry of the periodic structure is carefully examined in order to define the smallest elementary cell necessary to reproduce the infinite pattern and to avoid extended calculation time. For each wavelength the real and imaginary part of the dielectric function $n(\lambda)=n'(\lambda)+ik(\lambda)$ is taken into account. They correspond to the index of a P3HT: PCBM material, made of a classical blend of poly-3-hexylthiophene (P3HT) and [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). Fig. 1 shows the P3HT: PCBM index dispersion that we have used.

Absorption is then computed as the ratio between the energy that is lost for the electromagnetic wave (neither reflected nor transmitted), and the energy of the plane wave incident onto the device.

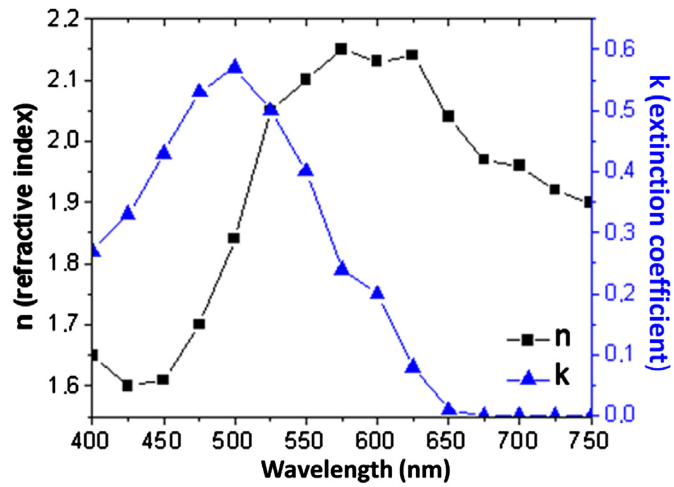

Fig. 1. Optical indices of P3HT: PCBM as a function of wavelength obtained by ellipsometry measurements.

3. Results and discussion

3.1. Properties of 2D PC in an absorbing slab

To understand the absorption enhancement induced by a 2D periodic array, we first study a simpler structure. It consists of a slab of P3HT: PCBM, in which a Photonic Crystal (air holes) has been patterned. A sketch of this device, that we now denote Photonic Crystal Slab (PCS), is shown in Fig. 2(a). Note that the full solar cell is studied in Section 3.2.

3.1.1. Frequential and temporal analysis of PCS

The PCS air holes, of radius $R=110$ nm, are positioned along a hexagonal lattice of period $a=500$ nm. The thickness of the layer, H, is 200 nm. We choose the axis x and y (see Fig. 2(a)) to be along two main directions of the hexagonal structure. Let us consider a plane wave, incident onto the PCS in the z direction, and linearly polarized. A priori, one can expect that the PCS optical response would depend on the polarization direction (by respect to x and y). As sunlight is unpolarized, and can be modeled as a superposition of linearly polarized fields in random directions, the actual optical response of a PCS to sunlight would be a randomly weighted sum of its response to linearly polarized light, at all the possible polarization angles. Hopefully, we have noticed that the absorption spectrum is almost the same; whether one imposes the incident E-field to be polarized along x or along y. Therefore, when computing absorption spectra, in the entire article, we have chosen to set the incident plane wave polarized along x. This simplifies the study, but the results remain meaningful in a realistic case.

The incident light is a TEM plane wave in normal incidence to the PC plane. The Fig. 2(b) compares the absorption spectrum of a PCS and of a planar reference slab which is not patterned. Both are of the same thickness and made of the same absorbing material. One observes, for the PCS, that a resonance at 638 nm appears, which is not present for the reference slab. Fig. 2(c) shows the map of the z-component of the Poynting vector at resonance.

At first sight, such observation seems to be a paradox. Indeed, at a particular wavelength, one observes a much stronger absorption in the PCS, where, however, a fraction of the P3HT: PCBM (absorbing material), has been removed and replaced by air (non-absorbing). A possible cause, to explain such difference, is that the presence of air holes distorts the wave front and increases the optical path followed by light when it passes through the slab. To